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Modeling Dispersion of Chemical-Biological Agents in Three Dimensional Living Spaces

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ABSTRACT

This report documents a series of calculations designed to demonstrate Sandia's capability in modeling the dispersal of chemical and biological agents in complex three-dimensional spaces. The transport of particles representing biological agents is modeled in a single room and in several connected rooms. The influence of particle size, particle weight and injection method are studied.

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Introduction

This report will present a series of calculations designed to demonstrate Sandia's capability in modeling the dispersal of chemical and biological agents in complex three-dimensional spaces.

Recent events have underscored the need to anticipate, prevent and mitigate the introduction of toxic chemical and biological (CB) agents into our living spaces. Most Americans spend approximately 90% of their time indoors in homes, offices and other public enclosures such as airports, shopping malls, subway stations, theaters and arenas. These inherently three-dimensional living spaces are made more complex due to the placement of doors, windows, vents, walls and furniture. Qualitative modeling of the flow of air and the transport of CB agents in such spaces is difficult, if not impossible to accomplish using network or zonal models that treat the space as a single control volume.

The dispersion of CB agents in large volumes is facilitated by forced convection from building heating, air conditioning, and ventilation (HVAC) systems. In addition, free convection resulting from thermal and solutal buoyancy often plays a role in spreading CB agents. Modeling the fluid dynamics of the carrier gas (ambient air) requires the multidimensional solution of the Navier-Stokes equations. When heat transfer is important the energy equation should also be included. Additional coupled equations must be solved depending on the CB threat. In the case of poison gas (e.g. sarin, phosgene, etc.) species equations must be solved. It may even be necessary to include complex models for multicomponent and thermal diffusion. Modeling the dispersion of aerosol biological agents (e.g. anthrax, smallpox, etc.) requires a particle tracking capability.

The calculations described here will focus on the dispersal of "anthrax-like" particles in large three-dimensional spaces. A set of "demonstration" calculations will be presented to show how computational fluid dynamics (CFD) can be used to determine the influence of room orientation, vent and door location, particle size, particle weight, and the method used to introduce the particles.

Previous Work

Sandia has engaged in activities for sensing, analyzing, and responding to CB threats (See *e.g.* [1]). The network flow modeling code, KBERT [2], has been used to model CB agent dispersal in large complex structures such as the Albuquerque Court House. Network flow codes such as KBERT rely on one-dimensional flow modeling with locally applied correlations to capture multidimensional behavior. Typically each room in a building simulation is modeled using a single control volume. For the Albuquerque Court House modeling work, larger rooms were subdivided into several control volumes in an attempt to improve resolution.

More recently, a series of tracer-gas release experiments was conducted at the International Terminal of the San Francisco International Airport to assess the impact of postulated CB agent terrorist attacks [3]. The study also attempted to identify responses that might mitigate such attacks. Several organizations played a role in these experiments including Sandia, Argonne National Laboratory, Washington State University, and Honeywell, Inc.

The Chemistry and Materials Processing Department at Sandia (Organization 8728) recently modeled the dispersal of toxic gas in three-dimensional space. This work [4,5] was performed to support Explosive Destruction System (EDS) testing for the Engineering Emerging Technologies Department (Organization 8118). Transient three-dimensional models were constructed to describe the dispersal of toxic phosgene gas resulting from a postulated "worst case" leak in the EDS device. The calculations accounted for three-dimensional solutal buoyancy effects and the influence of a ventilation flow field.

Modeling Approach

In our work we utilized the computer code CFX4.3 [5] to model the transport of particles in a carrier gas (atmospheric air). CFX is a three-dimensional transient and steady state CFD code with the following capabilities and characteristics:

- Finite volume code
- "Simple" based pressure/velocity coupling
- Multi-block, body fitted block structured grids
- Pre and post processing modules
- Incompressible and compressible flow (Ma<4.0)
- Laminar and Turbulent flow
- Multispecies transport and simple gas phase chemistry
- Two phase flow including Lagrangian particle tracking including buoyancy effects
- Addition features not pertinent to CB agent dispersal

The procedure for determining particle tracks may be summarized as follow:

1. The three-dimensional space was discretized (meshed) into suitable control volumes. For these demonstration calculations, all control volumes were cubes with six-inch sides.
2. The steady state flow field for ambient air and ventilation flow was calculated. The influence of thermal gradients on air motion was neglected but could have easily been added if it was deemed important.
3. Particle tracks were computed based on the assumption that the presence of the particles does not influence the flow field, i.e. there is only a one-way coupling to the particle transport. The airflow affects the particles, but the particles do not affect the

airflow. Complete (two-way) coupling can also be modeled for those cases when particle concentrations and sizes are large.

Momentum from the ambient airflow is imparted to particles via particle drag. Gravitational and particle drag forces ultimately determine the direction and speed of the particle. A number of particle drag models are available in CFX. The calculations performed here utilized the default CFX particle drag model that was formulated by Schiller and Nauman (1933). The particle drag coefficient is given by

$$C_d = \frac{24}{R_e}\left(1.0 + 0.15 R_e^{0.687}\right) \quad (1)$$

which is valid for particle Reynolds, R_e numbers in the viscous regime (R_e < 500-1000) where R_e is defined by,

$$R_e = \frac{r d \left|V_r\right|}{m}. \qquad (2)$$

In equation (2) r, m, d, V_r are the air density and viscosity, the particle diameter, and the relative velocity between the particle and the local surrounding air. Except near HVAC vent inlets, air velocities in rooms tend to be quite low (typically $V_r < V_{air} < 1$ m/s). This leads to relatively low particle Reynolds numbers so that Equation (1) reduces to the expression for Stokes flow, i.e.

$$C_d = \frac{24}{R_e}. \qquad (3)$$

Calculations

Calculations were made for particle transport in a single room and for multiply connected rooms. The ventilation flow rates for the calculations were provided by Sandia's Facilities Planning and Engineering Department, 8512, and are representative of typical building HVAC systems. Particle diameters of 1 micron (small particle) and 10 microns (large particle) were considered. These diameters bound the range of postulated weaponized anthrax particles. Two particle densities were considered, namely light particles having a density 0.1 times the density of water, and heavy particles having a density equal to water. Particles were introduced into the flow field in two different ways. For some calculations particles were carried into the room through inlet ventilation openings. In other calculations, particles were assumed to originate on a desktop to simulate what might happen if a letter containing an anthrax-like substance was opened in an office space. For this latter case, the particles were given some small initial velocity to lift them out of the desktop flow boundary layer. In some cases (*i.e.* large dense particles), the particles immediately settled back down on the desk, while in other cases the airflow in the room lifted the particle off the desk and permitted them to remain airborne for extended periods of time before exiting the room (through a door or exit vent).

Results from Single Room Calculations

Figure 1 shows a perspective view of the simulated space for the "single room" calculations. The room is 20 by 20 feet with an 8-foot ceiling and a door, which is either opened or closed. The windows in the room play no roll in these calculations but could have been used to provide additional outflow boundaries or surfaces of elevated or lowered temperature depending on the conditions outdoors. An inlet ventilation flow of 500 CFM was provided through a ceiling vent near the right front of the room. Inlet flow was directed at a 45 degree down angle toward the center of the room. An exit flow vent was placed in the ceiling near the rear of the room on the left side. In all cases considered here, particles were introduced at the desktop near the rear of the room.

Figure 2 illustrates computed particle motions for lightweight particles (10% water density). Both small (1 micron) and large (10-micron) particles became airborne for extended periods of time before exiting through the open door. Particle flight times for the small and large particles were 1101 and 416 seconds respectively.

Figure 3 illustrates computed particle motions for heavyweight particles (water density). In this case only the 1-micron particle became airborne for several revolutions of the room before exiting through the open door (flight time 508 seconds). The 10-micron, heavyweight particle settled back down on the desk and did not become airborne.

Figure 4 shows computed lightweight particle trajectories for the single room with the door closed. Here again both the small and large particles became airborne before exiting the room through the ceiling exhaust vent. Flight times for the small and large particles were 329 and 267 seconds respectively.

High-density particle trajectories in the single room with the closed door are shown in Figure 5. As with the open door case, the 10-micron, heavyweight particle failed to become airborne. The small particle made several revolutions of the room and remained airborne for 872 seconds before exiting the ceiling exhaust vent.

Results from Three Room Calculations

Figure 6 shows a top view of a three-room office complex. The inlet and exhaust vents shown are all in the ceiling. The inlet flow direction is indicated by the shaded "plumes". All inlet flows are 250 CFM with a 30-degree down angle. The large (30 by 15-ft.) room contains a desk and an open door to an outside hallway. The large room is connected to two smaller (15 by 15-ft.) rooms by two open doorways.

Figure 7 shows the computed path of a 1-micron lightweight particle injected at the ceiling vent on the right hand side of the large room. The particle makes several revolutions of the large room, enters one of the smaller rooms for several revolutions, and then returns to the larger room before exiting through the door to the hallway. The total particle flight time was 1579 seconds.

Figure 8 shows the computed path of a 1-micron lightweight particle injected at the ceiling vent of the small room on the right. After injection the particle quickly moves into the large room where it is re-entrained into inlet vent flows and accelerated for an extended journey before exiting the hallway door. Total flight time for the particle was 3214 seconds.

Trajectories shown in Figures 9 and 10 are for small and large lightweight particles originating on the desk. The small particle shown in Figure 9 remains airborne in the large room for a period of 2141 seconds before exiting the hallway door. The larger particle flight time (Figure 10) was considerably shorter, *i.e.* 757 seconds.

Conclusions

The calculations described here were intended to demonstrate an ability compute flow fields and particle tracks in relatively complex multidimensional spaces. The study was not intended to lead to a comprehensive set of conclusions regarding generalized particle flow. Nevertheless some observations are apparent.

1. "Anthrax-like" bio agents less than 10 microns can remain airborne for extended time periods regardless of the method of introduction (desktop or vent flow).
2. Particles exit rooms through large open doorways rather than normal HVAC exhaust vents.
3. Particle trajectories and flight times are influenced by a number of factors including room design and orientation, HVAC configuration, and particle size and weight. Without some detailed multidimensional calculations, particle behavior would be difficult to anticipate using "common sense" or lower fidelity models.

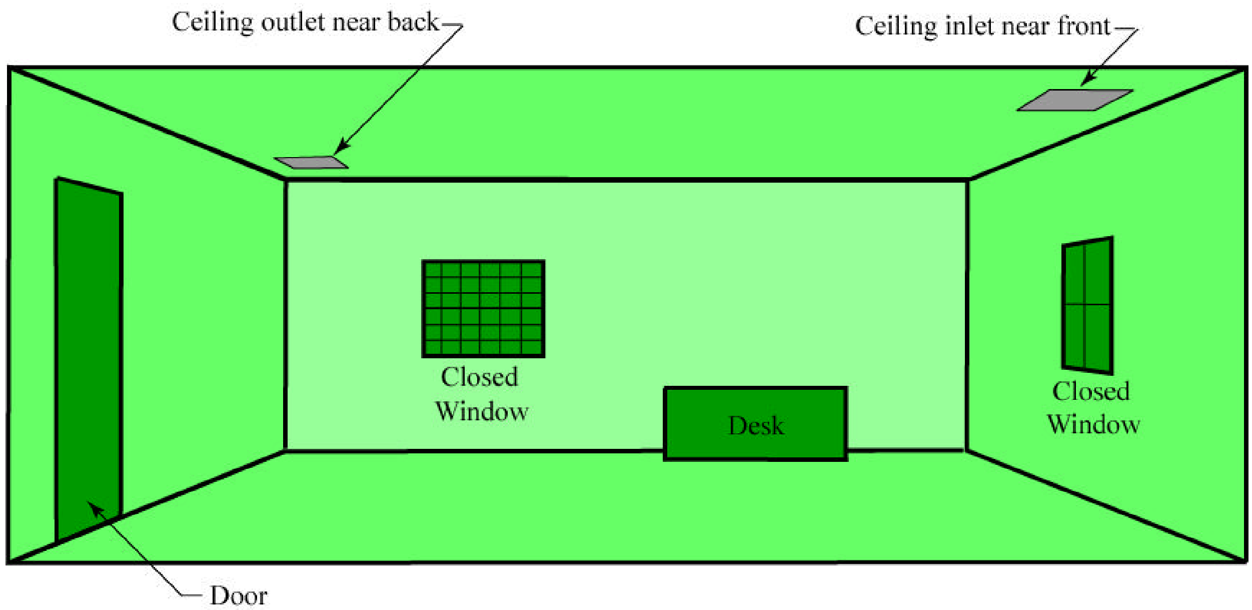

Figure 1. Single room orientation. 20 X 20 room, 8 ft high.

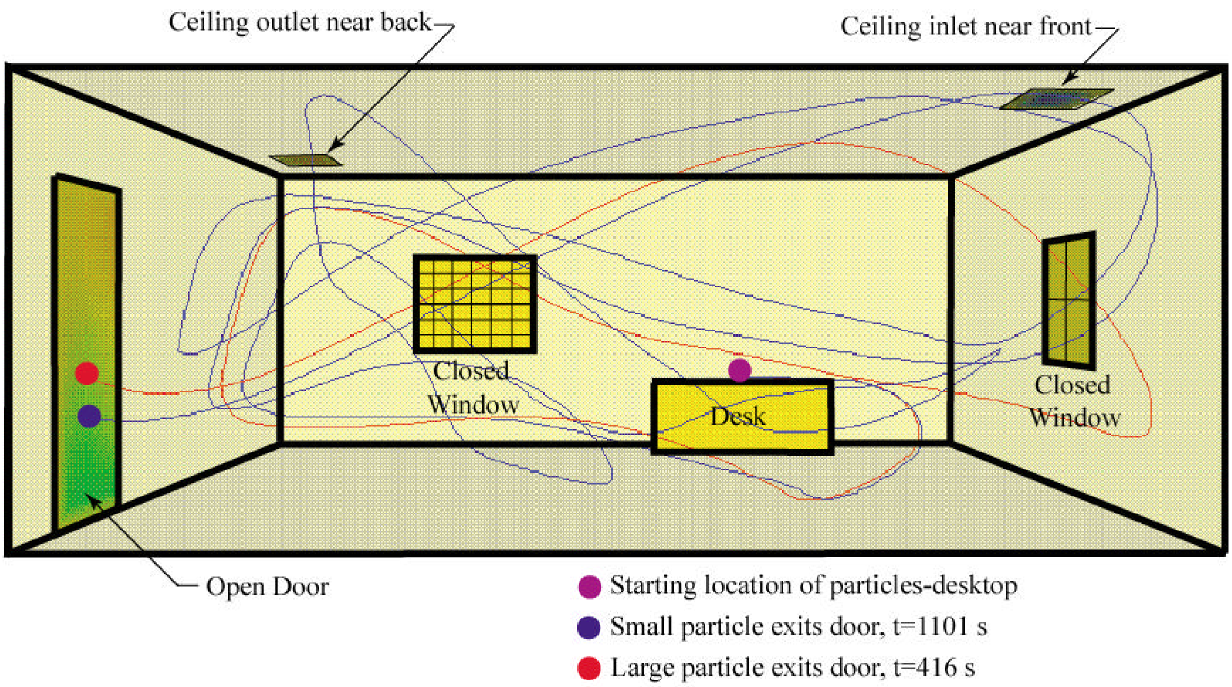

Figure 2. Low density particle trajectories in a single room (open door).

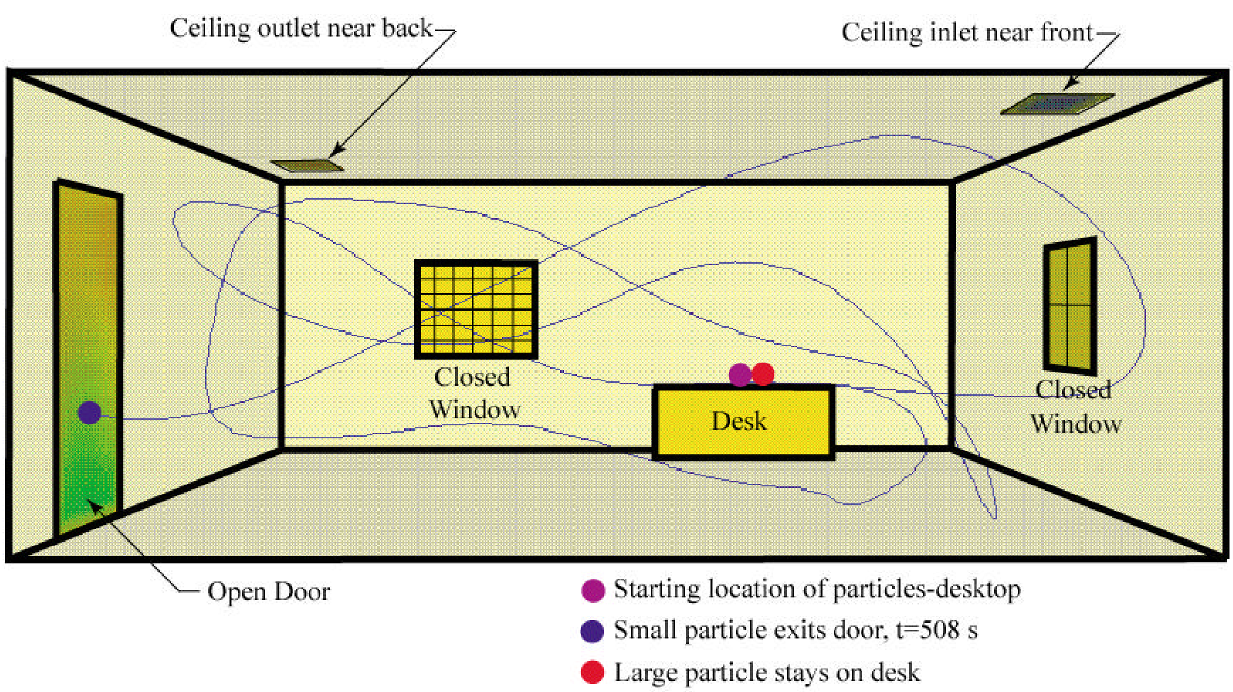

Figure 3. High density particle trajectories in a single room (open door).

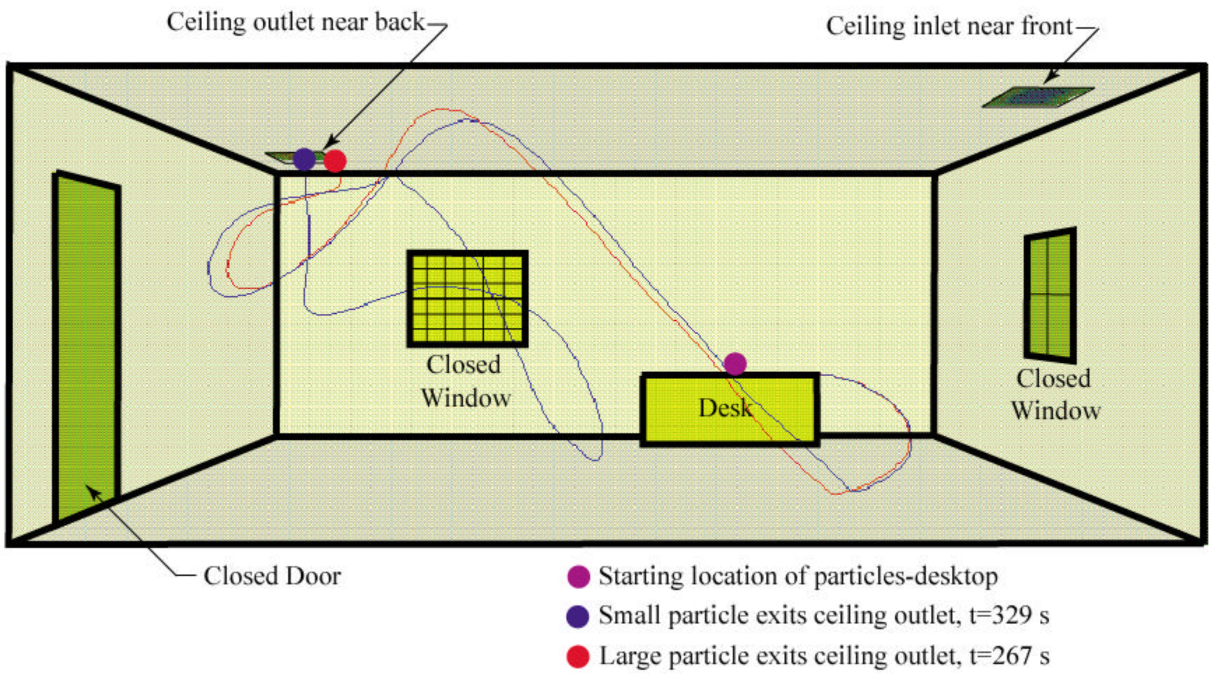

Figure 4. Low density particle trajectories in a single room (closed door).

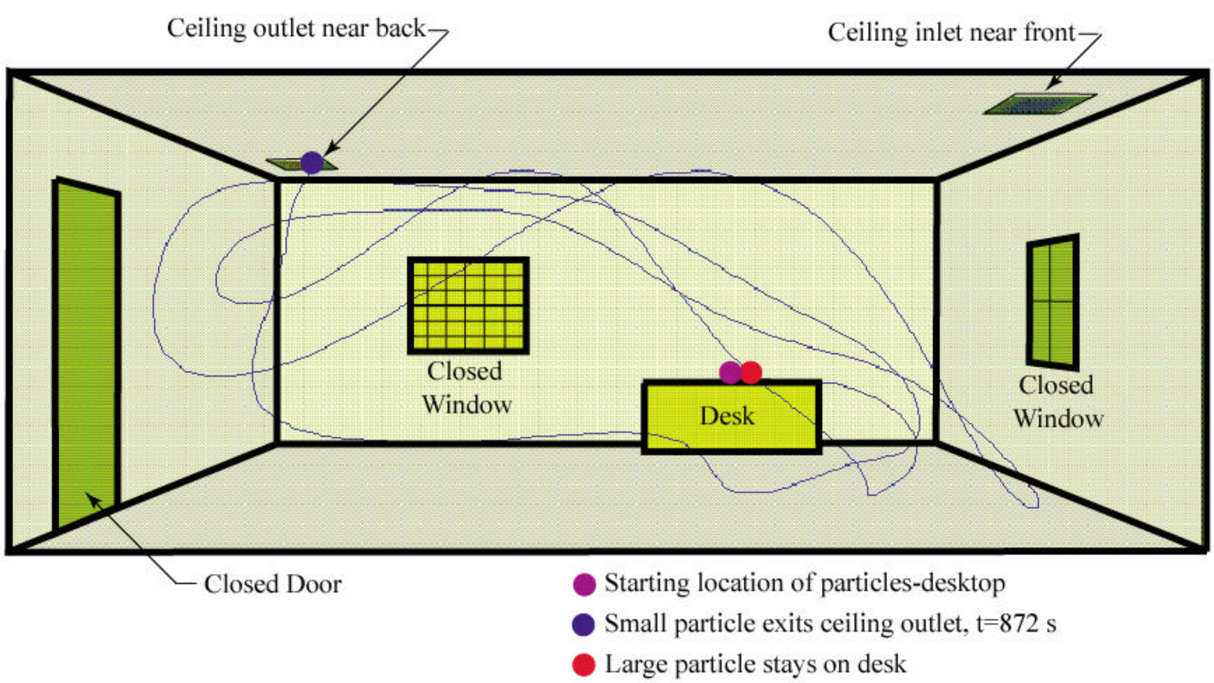

Figure 5. High density particle trajectories in a single room (closed door).

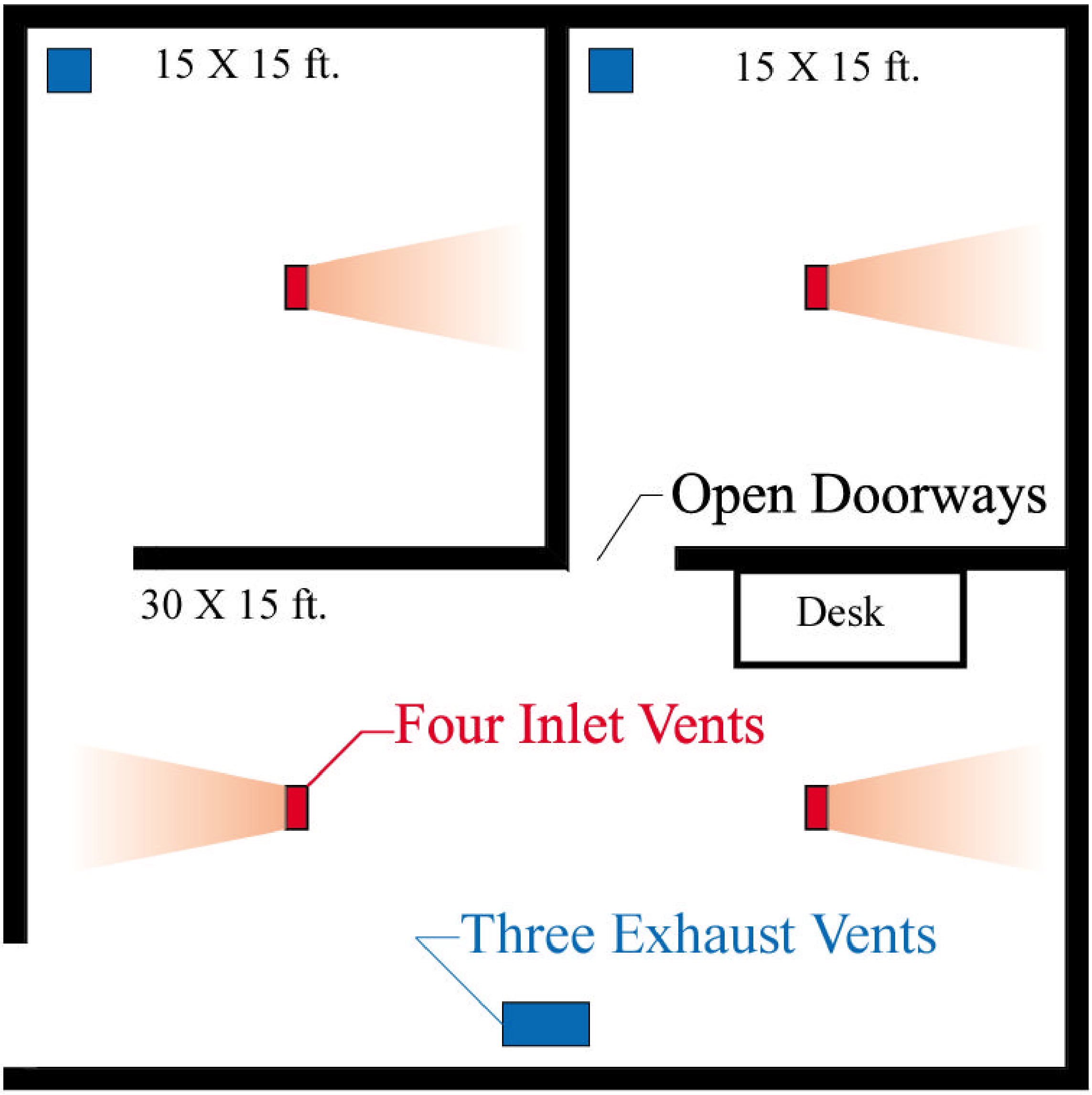

Figure 6. Three room office complex with 9 foot ceilings.

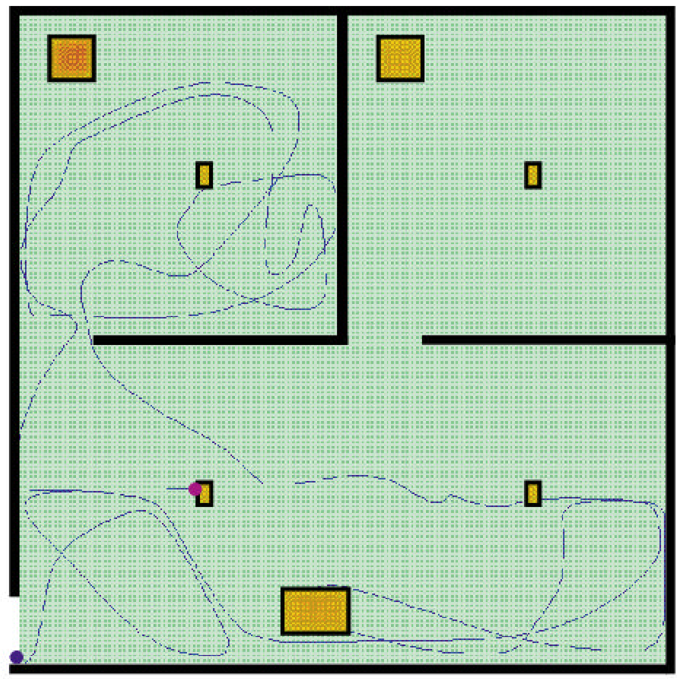

Figure 7. Small particle trajectory after injection from large room vent.

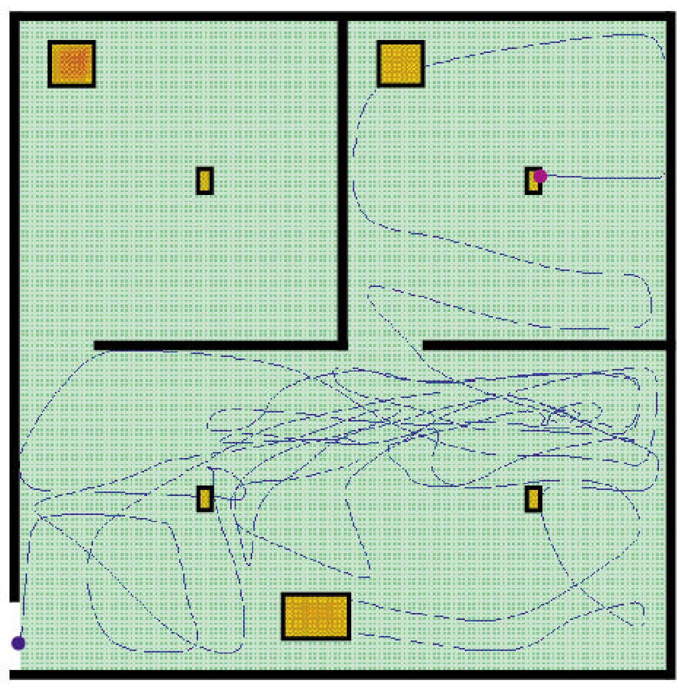

Figure 8. Small particle trajectory after injection from small room vent.

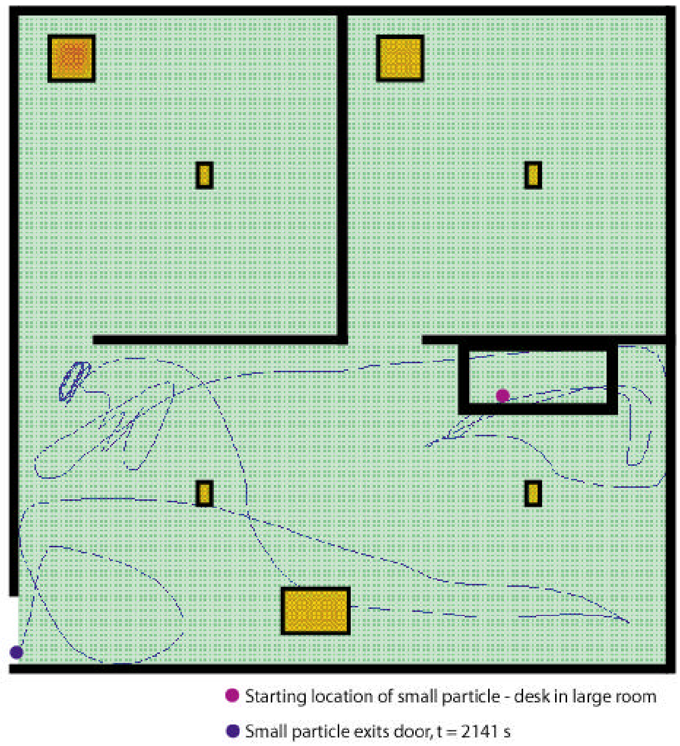

Figure 9. Small particle trajectory after being airborne from desk.

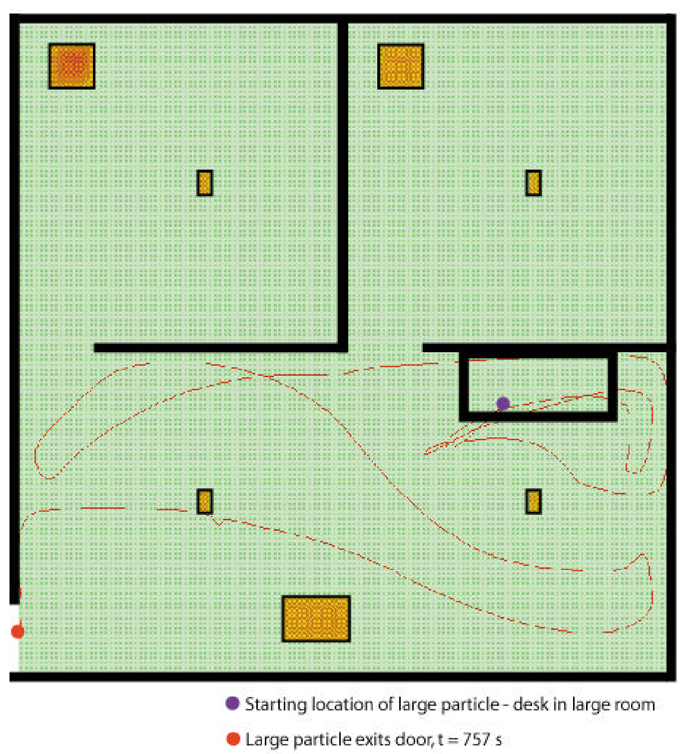

Figure 10. Large particle trajectory after being airborne from desk.

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